

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043025\
 Data File : BM050045.D
 Acq On : 30 Apr 2025 14:46
 Operator : RC/JU
 Sample : Q1883-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OU4-PCS-TC-28-042325

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	317	323	334	rBV	399493	587731	3.62%	0.841%
2	5.352	396	402	424	rBV	3986485	6232620	38.37%	8.921%
3	6.946	664	673	696	rBV	3688846	6419142	39.52%	9.188%
4	7.763	801	812	824	rBV	880006	1416995	8.72%	2.028%
5	8.922	998	1009	1032	rBV	2192319	4012899	24.71%	5.744%
6	10.563	1280	1288	1302	rBV	855053	1741842	10.72%	2.493%
7	13.028	1699	1707	1727	rBV	7012645	10554259	64.98%	15.107%
8	14.410	1932	1942	1955	rBV	1571178	2499538	15.39%	3.578%
9	15.769	2167	2173	2189	rBV	1657183	2386775	14.69%	3.416%
10	15.904	2189	2196	2218	rBV	5417651	8081088	49.75%	11.567%
11	16.333	2264	2269	2282	rVB	206821	322983	1.99%	0.462%
12	17.157	2402	2409	2424	rBV	1740792	2756961	16.97%	3.946%
13	18.051	2556	2561	2571	rBV	230685	428302	2.64%	0.613%
14	18.909	2700	2707	2715	rBV4	80564	205003	1.26%	0.293%
15	19.780	2849	2855	2866	rBV	14300293	16242834	100.00%	23.249%
16	21.068	3071	3074	3085	rVB2	190809	353400	2.18%	0.506%
17	21.398	3125	3130	3142	rVB	1780437	2736548	16.85%	3.917%
18	24.397	3632	3640	3661	rVB	1047111	2884296	17.76%	4.128%

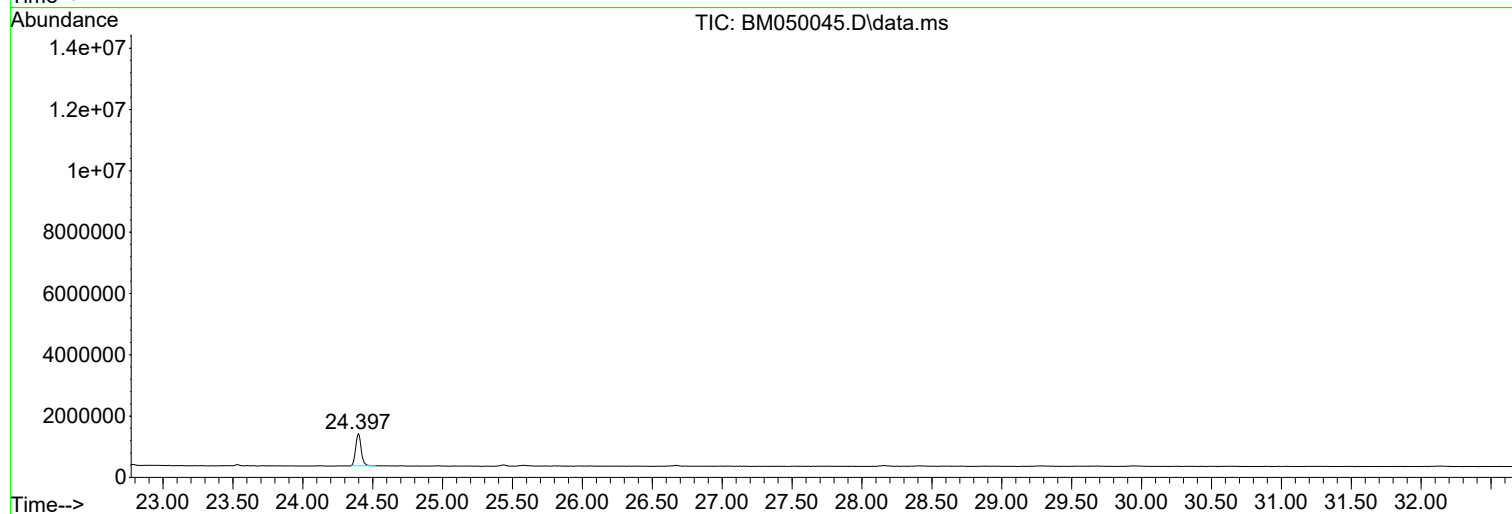
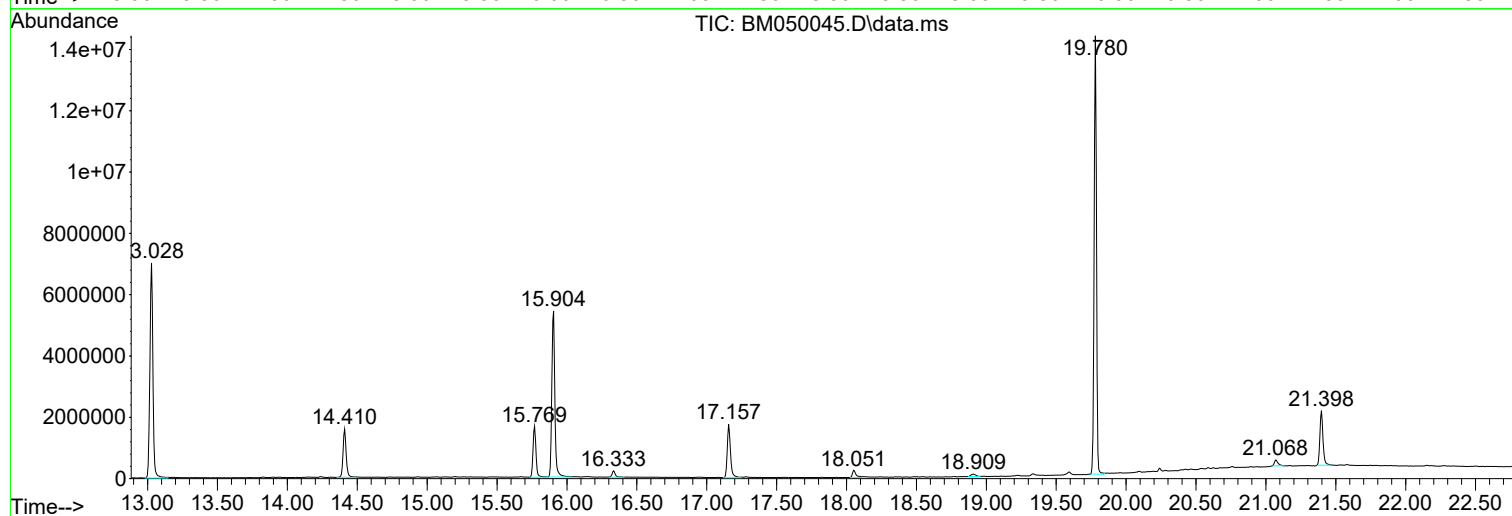
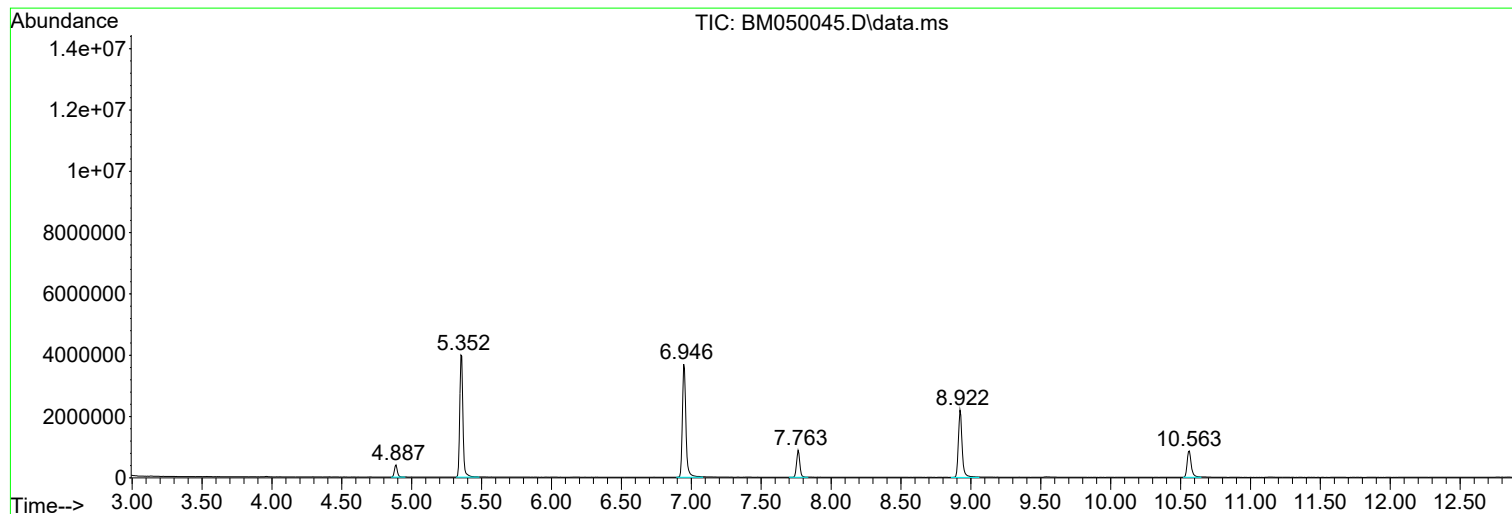
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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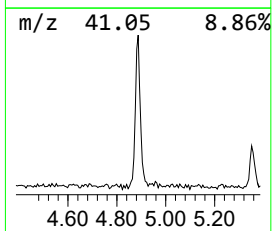
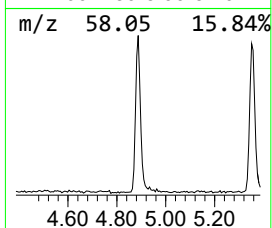
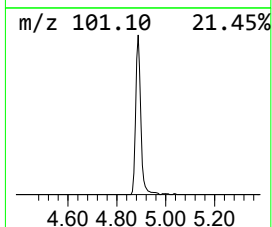
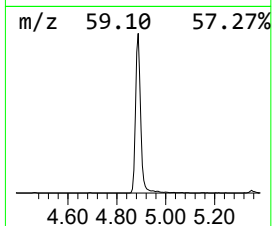
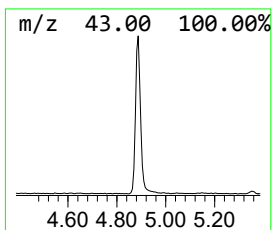
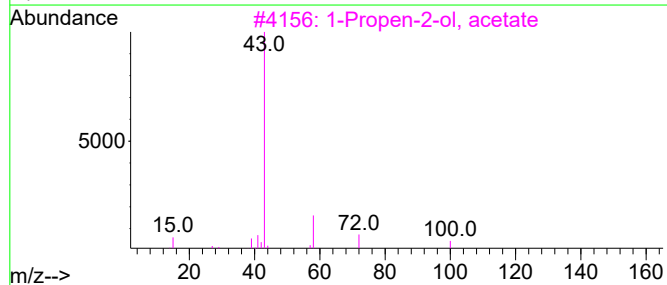
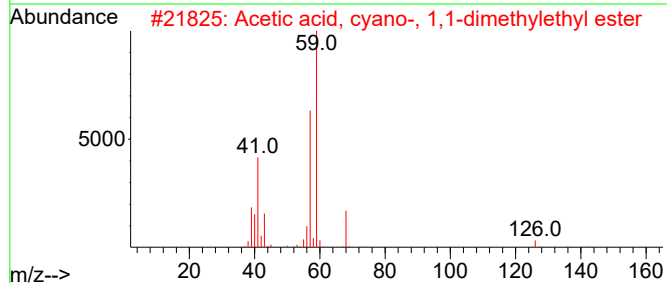
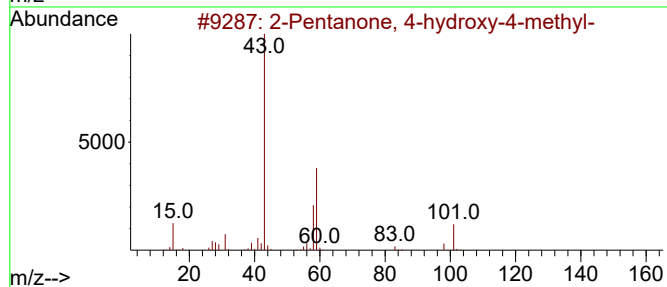
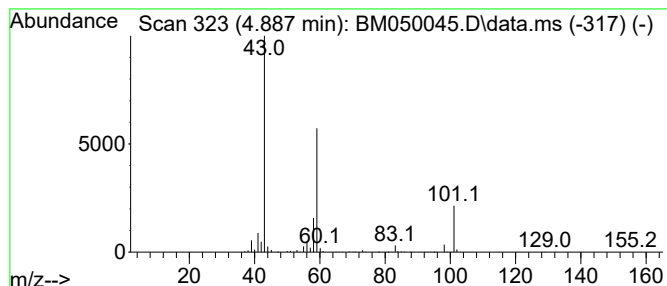
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	8.30 ng	587731	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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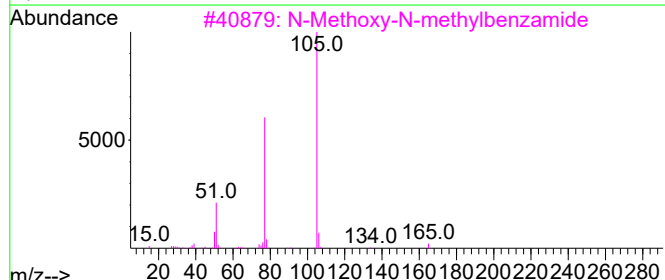
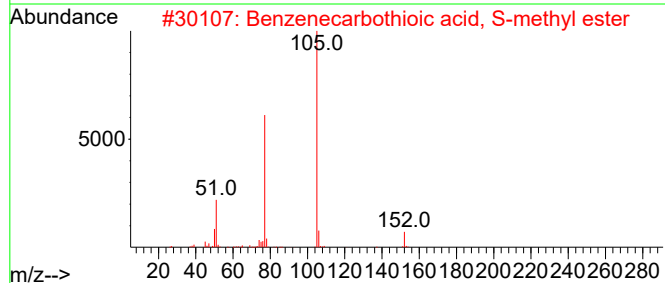
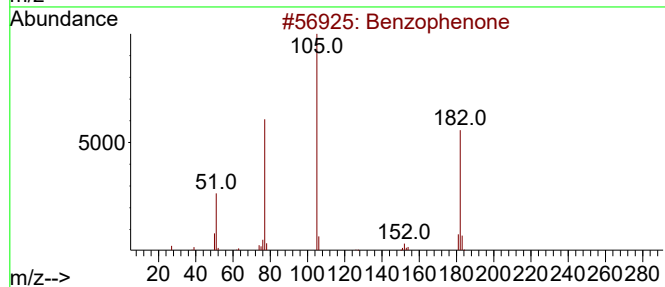
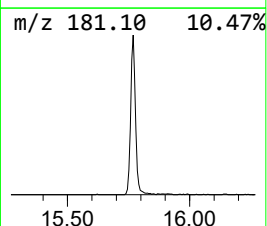
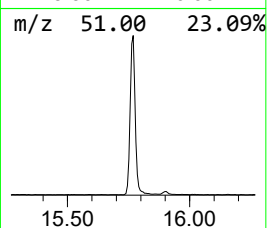
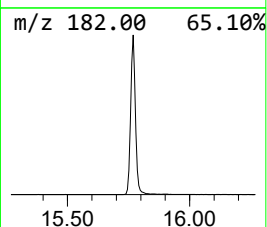
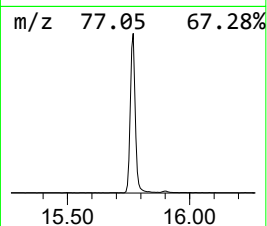
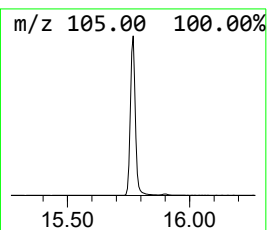
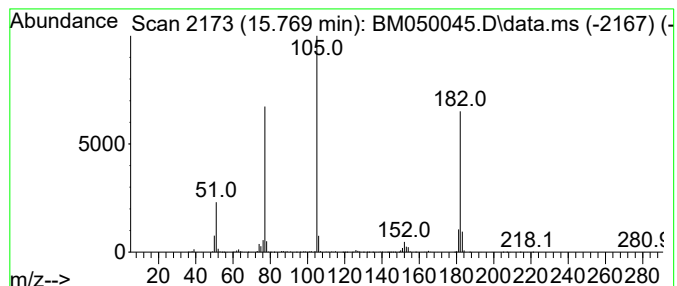
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.769	19.10 ng	2386780	Acenaphthene-d10	14.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43



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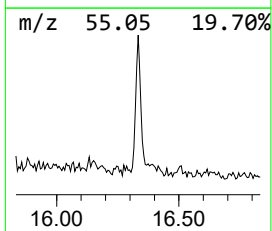
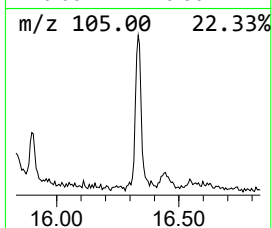
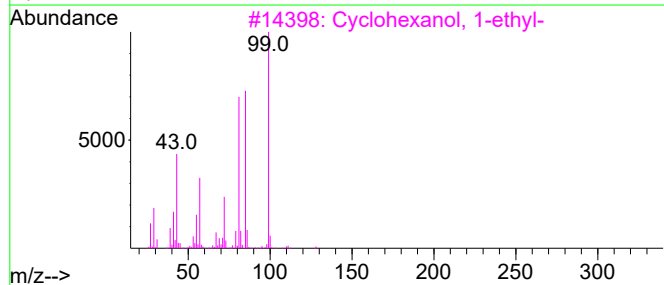
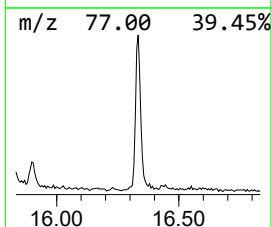
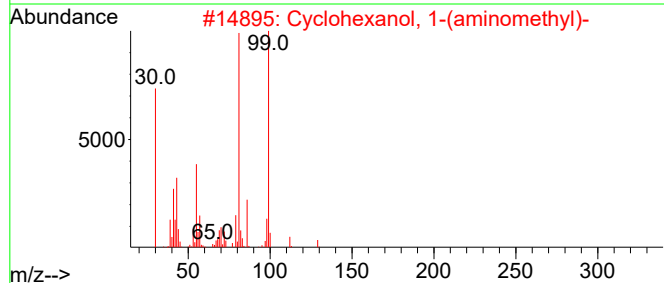
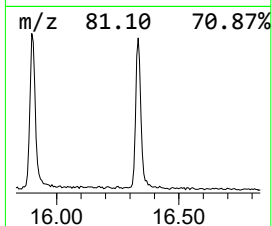
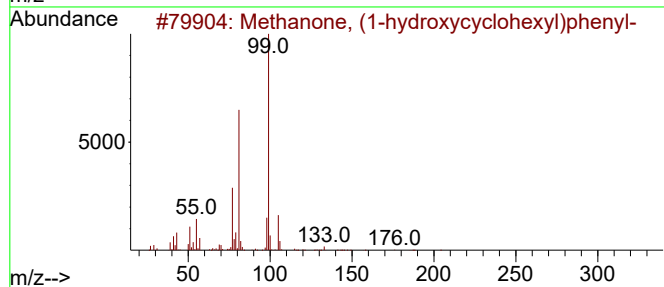
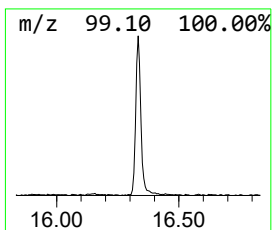
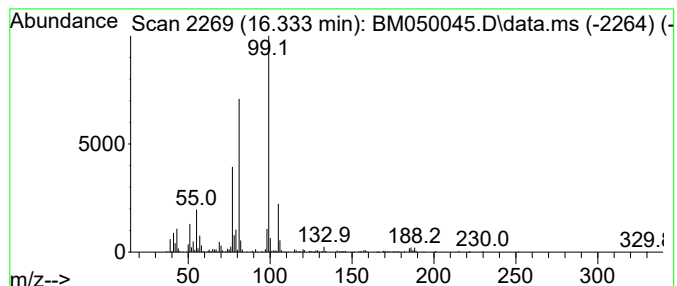
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	2.34 ng	322983	Phenanthrene-d10	17.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	87
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	47
3			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	43
4			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	37
5			2-(1-Hydroxycyclohexyl)butanoic ...	186	C10H18O3	000512-16-3	37



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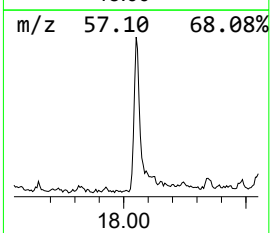
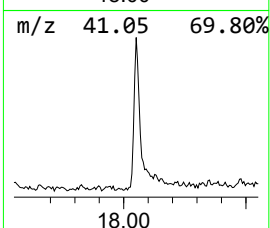
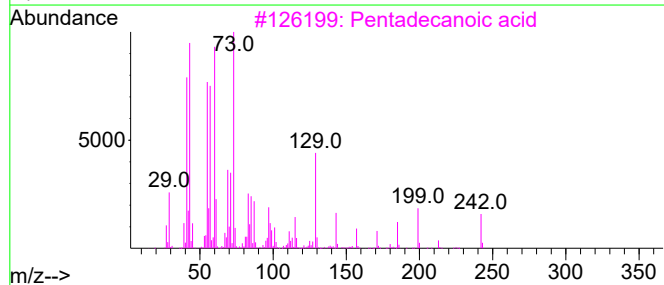
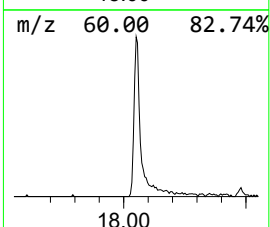
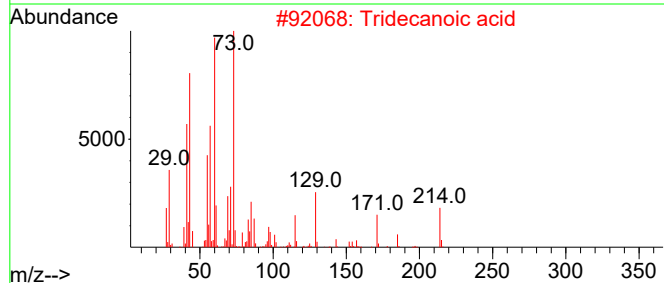
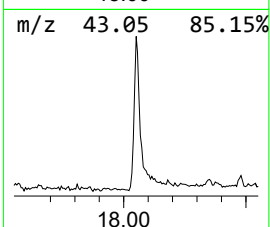
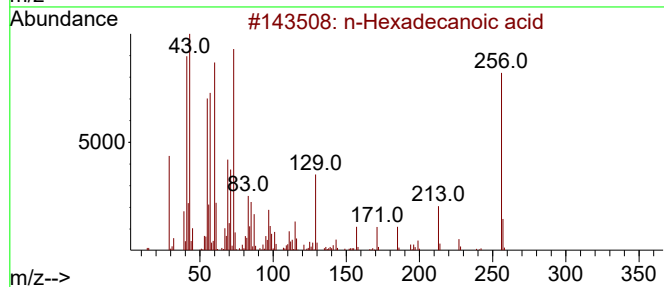
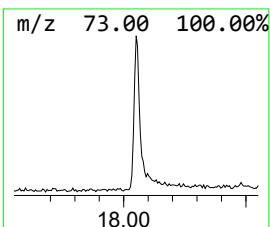
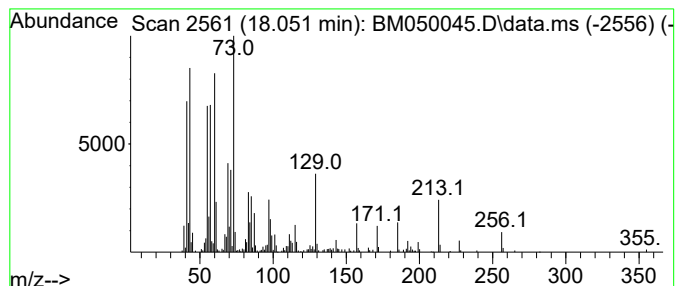
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	3.11 ng	428302	Phenanthrene-d10	17.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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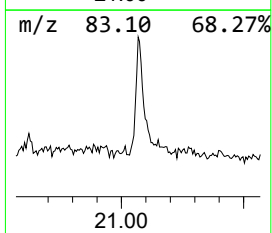
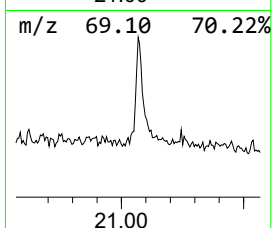
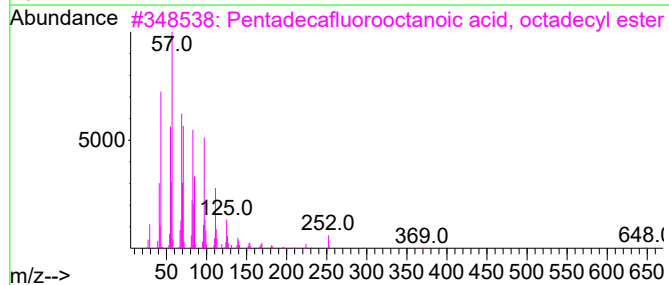
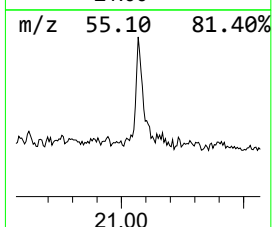
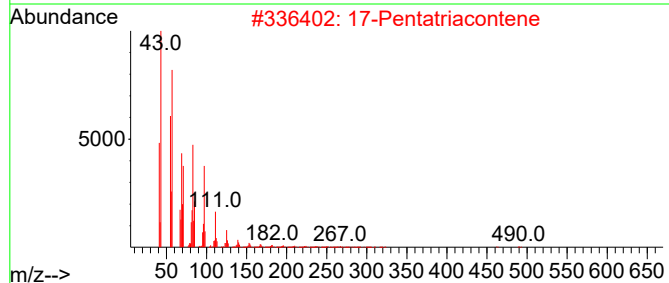
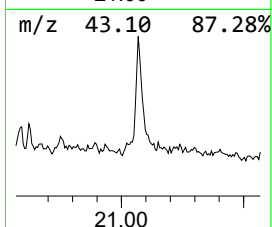
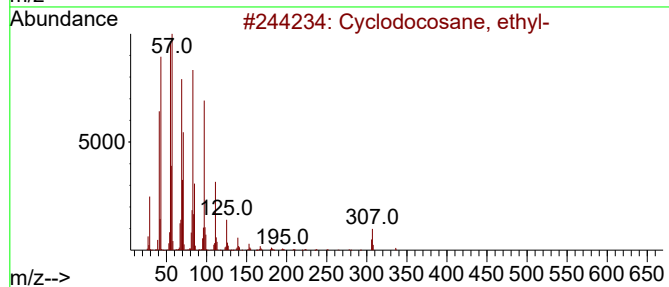
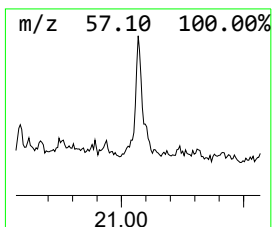
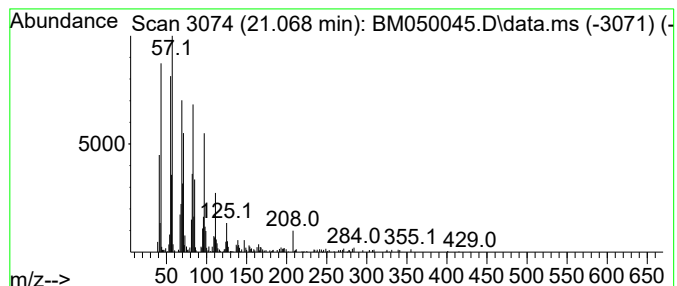
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Peak Number 5 Cyclodocosane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.068	2.58 ng	353400	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.887	8.3	ng	587731	1	7.763	1417000	20.0
Benzophenone	15.769	19.1	ng	2386780	3	14.410	2499540	20.0
Methanone, (1-h...	16.333	2.3	ng	322983	4	17.157	2756960	20.0
n-Hexadecanoic ...	18.051	3.1	ng	428302	4	17.157	2756960	20.0
Cyclodocosane, ...	21.068	2.6	ng	353400	5	21.398	2736550	20.0